CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES QUALITY ASSURANCE PROCEDURE	Proc. QAP-014 Revision 2 Chg 2 Page 1 of 4

Title QAP–014 DOCUMENTATION AND VERIFICATION OF SCIENTIFIC AND ENGINEERING CALCULATIONS

EFFECTIVITY AND APPROVAL

Revision 2 of this procedure became effective on 8/30/2000. This procedure consists of the pages and changes listed below.

Page No.	Change	Date Effective
All	2	7/28/2004

Change 2 incorporates editorial changes and uses the term Manager instead of Element Manager.

Supersedes Procedure No. QAP–014, Rev. 2 Chg 1, dated 8/30/2000.

Approvals

Written By	Date	Concurrence Review	Date
/s/Robert Brient	7/30/2004	/s/English Pearcy	8/2/2004
Quality Assurance	**Date**	**Cognizant Director**	**Date**
/s/Mark R. Ehnstrom	7/30/2004	/s/Patrick Mackin	8/2/2004

CNWRA FORM QAP-1 (12/92)

QAP–014 DOCUMENTATION AND VERIFICATION
OF SCIENTIFIC AND ENGINEERING CALCULATIONS

1. PURPOSE

The purpose of this procedure is to specify the methods for documenting and verifying scientific and engineering calculations. This procedure applies to calculations performed by hand, hand calculator, and by computer software.

2. RESPONSIBILITIES

2.1 The investigator is responsible for documenting calculations in a scientific notebook as specified in this procedure.

2.2 Technical reviewers are responsible for verifying samples of calculations as specified in this procedure.

3. PROCEDURE

3.1 Documentation of Calculations

Calculations shall be sufficiently documented in appropriate scientific notebooks or in the reviewed document itself sufficiently so that they can be duplicated.

3.1.1 Data inputs and computational methods shall be documented as follows:

(i) Calculations Performed Using Controlled Software – The name and version number of the controlled software and the input files will submitted as part of the QA records for a document.

(ii) Calculations Performed Using Uncontrolled Software – A source code or an executable copy of the uncontrolled software together with the input file will be submitted as a part of the QA records for a document.

(iii) Calculations Performed Using Commercial-off-the-Shelf Software – The name and version number of the commercial-off-the-shelf software (e.g., spreadsheets, Mathematica, Mathcad) source code for any macros formulae, or script, and the input data will be submitted as a part of the QA records for a document.

(iv) Other Calculations – A description of the calculation method, in detail sufficient for reapplication, and the data used will be submitted as a part of the QA records for a document.

3.1.2 Output data from calculations shall be documented in the scientific notebook. If the output data consist of large files, the files may be copied to a disk and attached to the scientific notebook, or the scientific notebook may reference a file location. Electronic output files should identify the software name and version and date of the calculation. When complete input files are included in the QA records, only a sample of the output files is required.

3.2 Verification of Calculations

The objective of the verification of calculations is to assure their arithmetic correctness. In consultation with the author(s), the manager responsible for the document will determine whether a CNWRA product contains calculations and the extent to which these calculations require verification. The manager will make this decision based on (i) potential importance of the calculations with respect to their intended use, (ii) extent of prior verification in related reports or papers, and (iii) complexity of calculation and potential for errors. For calculations performed using controlled software, verification of input data is generally sufficient. For calculations performed using uncontrolled software, a check of output using alternate software or hand calculations of a subset of the analysis will generally also be required. For calculations performed using commercial-off-the-shelf software (e.g., spread sheets, Mathematica, Mathcad), verification of a suitable number of formulae will generally be required in addition to the foregoing checks of input and output. The manager will note on the Instructions to Technical Reviewers (CNWRA QAP–12–4 Form) the extent and type of over checks required and obtain concurrence of the Technical Director for the same. When calculation over checks are not performed, a rationale shall be provided.

In verifying calculations, the assigned reviewer will obtain access to relevant scientific notebooks and records of input and output data files, as appropriate. The reviewer may require access to the software, if any, and exercise it as a part of the verification process.

3.2.1 The reviewer shall verify that input data have been documented as required in paragraph 3.1.1.

3.2.2 The reviewer shall verify that the calculation methods have been documented as required in paragraph 3.1.1.

3.2.3 The reviewer shall verify that output data has been documented as required in paragraph 3.1.2.

3.2.4 The reviewer shall verify the calculations to the extent determined by the manager as follows.

(i) Calculations Performed Using Controlled Software – Check a sample of the input data to determine that data are correctly entered and are free of errors (e.g., incorrect units, misplaced decimal, incorrect exponent, value in the wrong field, etc.). Check a sample of the output for reasonableness.

(ii) Calculations Performed Using Uncontrolled Software – In addition to checks in (i), verify sample results by alternate calculations either by hand by using alternate software, or by reviewing the basic logic of the uncontrolled software. The reviewer may ask the assistance of the author(s).

(iii) Calculations Performed Using Commercial-off-the-Shelf Software – Check a sample of the formulae employed , the correctness of a sample of the input data, and the reasonableness of a sample of the output.

(iv) Other Calculations – Check correctness of a sample of the input data and verify sample results by alternate calculations.

3.2.4 Verification of calculations will be documented as part of the reviewer comments on the CNWRA TOP–3 Form. The reviewer shall indicate how the sample verification was accomplished and the conclusions regarding the correctness of calculations. For example, the reviewer may state that the document under review used xxx software(s), which is controlled/uncontrolled, a sample of the input data recorded within the report or in Scientific Notebook No. yyy was checked, and an alternate calculation was/was not performed. The check determined that the calculations were/were not performed correctly.

3.2.5 In case errors are found, the author(s) must obtain resolution with the reviewer before the product can be released.

4. RECORDS

Technical review comment resolution sheets shall be retained as QA records in accordance with QAP–012, Quality Records Control.